







an Open Access Journal by MDPI

New Insights into Machine Learning in Chemistry, Biochemical Engineering, and Pharmacy

Guest Editors:

Prof. Dr. Mia K. Markey

1. Department of Biomedical Engineering, The University of Texas at Austin, Austin, TX 78712, USA

2. Department of Imaging Physics, The University of Texas MD Anderson Cancer Center, Houston, TX 77030, USA

Dr. Yao Zhang

Expedia Group, 1111 Expedia Group Way W, Seattle, WA 98119, USA

Deadline for manuscript submissions:

closed (30 June 2022)

Message from the Guest Editors

Recent advances in machine learning have sparked enthusiasm for applications in chemistry and allied disciplines such as biochemical engineering and pharmacy. There are numerous opportunities for machine learning to support the chemical sciences, but it is important to distinguish between advances in current practice and potential future benefits of these technologies. Scientists, engineers, and clinicians need to know both how they can leverage machine learning in its present state and what the prospects are for future utility in chemistry and allied disciplines.

The aim of this Special Issue is to present recent advances in machine learning applications in the fields of chemistry, biochemical engineering, and pharmacy. Reviews, full papers, and short communications, from methodological advances to healthcare implications of current trends in machine learning applied to chemistry and allied disciplines, are all welcome.













an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

Author Benefits

Open Access: free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility: indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.

Journal Rank: JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Contact Us